



EPA

USAGE OF COMPUTER MODELS IN THE HAZARDOUS WASTE AND SUPERFUND PROGRAMS

REVIEW OF OSWER'S DRAFT REPORT ON THE USAGE OF COMPUTER MODELS IN- THE HAZARDOUS WASTE/SUPERFUND PROGRAMS AND PROPOSED PILOT STUDY



UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

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September 6, 1991

OFFICE OF
THE ADMINISTRATOR

Honorable William K. Reilly
Administrator
U.S. Environmental Protection Agency
401 M Street, S.W.
Washington, D.C. 20460

Dear Mr. Reilly:

The Science Advisory Board (SAB) has completed its review of the Office of Solid Waste and Emergency Response (OSWER) draft report entitled "Report on the Usage of Computer Models in Hazardous Waste/Superfund Programs," dated November, 1990, and the proposed OSWER pilot study on model management. The report and proposed pilot project were reviewed and discussed in a teleconference review meeting on December 7, 1990, at which time Subcommittee members conveyed comments to representatives of OSWER's Information Management staff, their contractor and personnel from the EPA Office of Research and Development (ORD).

The Subcommittee finds that the study presented in the draft report was well planned and executed, and was very responsive to the issues raised in the SAB Modeling Resolution. The conclusions drawn in the report are consistent with the data and information presented. Needs for some improvements to the draft report were identified; in particular, the OSWER staff should review the list of models for accuracy of classifications and names, especially where some models are known by multiple names. We also recommend that follow-up work be conducted to improve the overall value of the study. This follow-up work should include the following:

- a. Several case studies illustrating how models were used and applied by EPA personnel,
- b. The models listed in the report should be identified and categorized according to their primary function. This would complement: the information provided in the report on the use of the various models in different phases of RCRA and Superfund activities, and
- c. Further consideration should be given to the different levels of education and training needed for different modeling tasks, such as model development, model use, and review of modeling results of others. The pilot study on model management originally proposed by OSWER was to involve soil contamination models. The Subcommittee felt that the science of



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processes affecting soil contamination is not well understood, and that corresponding models are still very much in the research phase. Thus, it would be difficult to obtain what constitutes an acceptable model or set of models for soil pollution problems. As an alternative, the Subcommittee suggested that OSWER consider a study on the use of ground water flow models with possible extension to solute transport models applied to the saturated zone. Ground water flow models have been used in a wide range of applications for a number of years, and several good models are widely accepted as standard tools. The Subcommittee believes that such a study would allow a clearer focus to be placed on the administrative aspects of model management, including procedures for determining whether a model is acceptable for use in a particular application, establishing protocols for proper model validation and application, and mechanisms for education, information dissemination and model user support.

These recommendations are made with the anticipation that OSWER's models management initiative will be encouraged within the Agency. Further, the Subcommittee strongly supports the initiative taken by the OSWER Information Management staff to extend the OSWER activity Agency-wide with a proposed Agency Task Force on Modeling. The SAB views this initiative to be very important, as its proper implementation should lead to the eventual establishment of a formal institutional mechanism with responsibility for review, oversight and coordination of model use within the Agency.

We are pleased to have had this opportunity to be of service to the Agency, and look forward to your response to this report.

Sincerely,


Raymond C. Loehr, Chairman
Executive Committee
Science Advisory Board


Richard A. Conway, Chairman
Environmental Engineering Committee
Science Advisory Board


Mitchell J. Small, Chairman
Modeling Project Subcommittee
Science Advisory Board

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ABSTRACT

The Modeling Project Subcommittee (MPS) of the Environmental Engineering Committee (EEC) of the EPA Science Advisory Board (SAB), has reviewed aspects of the Office of Solid Waste and Emergency Response (OSWER) models management initiative. The review examined OSWER's draft report entitled, "Report on the Usage of Computer Models in Hazardous Waste/Superfund Programs," and a proposed OSWER pilot study on model selection and administration.

The MPS found that the study presented in the draft report was well planned and executed, and was very responsive to the issues raised in previous SAB reviews and resolutions. The conclusions drawn in the report are consistent with the data and information presented. The MPS suggested a number of improvements to the draft report, particularly regarding the accuracy of models listed and the use of multiple names for a given model.

Also, follow-up studies were recommended, involving case studies of model use in OSWER programs and further consideration of the types of training and education that are appropriate for different modeling activities.

The MPS found that the proposed OSWER pilot study on soil contamination models, while addressing an issue of great concern to the Agency, was probably not well suited as a test case for examining issues in model administration, due to the significant scientific uncertainty and research nature of these models. Rather, a project in a more established modeling domain, such as ground water flow models, was suggested to allow the study to focus better on administrative issues related to model selection and use at EPA.

The MPS strongly supports the model management initiative taken by the OSWER Information Management staff, and endorses extension of the activity Agency-wide through an Agency Task Force on Modeling.

Key Words: Mathematical Models, Superfund, CERCLA, RCRA, Computer Model Validation, Ground Water Models, Soil Contamination

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1. EXECUTIVE SUMMARY

This report provides a review of the EPA Office of Solid Waste and Emergency Response (OSWER) draft "Report on the Usage Of Computer Models in Hazardous Waste/Superfund Programs," and consultative comments on a proposed OSWER pilot study on model management. The proposed pilot study will identify a group of models which serve a particular function and determine the criteria which would qualify them as acceptable for use in EPA programs. This review was conducted by the Modeling Project Subcommittee (MPS) of the Environmental Engineering Committee (EEC) of the EPA Science Advisory Board (SAB).

The MPS found that the draft "Report on the Usage of Computer Models in Hazardous Waste/Superfund Programs," represents a very well-planned and executed study of model use in OSWER Programs. Recommendations to improve particular aspects of the report were made, including: inclusion of a summary of the Phase I report (the MPS reviewed only the second phase of the OSWER study); review of the list of models in the report for accuracy of classifications and names of models; and, clarification of the assertion that there is some, though little, model misuse in the OSWER programs. Suggestions were also made for additional work to enhance the study, including: presentation of extended case studies of model use in the OSWER programs; and, further consideration of the types of training and education that are appropriate for different modeling activities, including model development, model use, and review of modeling results developed by others.

Recommendations on the proposed pilot project were made with the understanding that these would depend on the goals and priorities of OSWER in conducting the study. These goals required further clarification. The initial proposal to study soil contamination models addressed a problem area of great interest to the Agency, but required a focus on scientific rather than administrative issues. Important administrative issues that should be addressed in the pilot study include the development of procedures to determine whether a model is acceptable for use in a particular application, establishing protocols for proper model validation and application, and mechanisms for personnel education, information dissemination and model user support. An alternative project in a more established modeling domain, such as ground water flow models, was thus suggested by the MPS to allow the study to focus better on these administrative issues related to model selection and use at EPA.

The MPS and the ETC is pleased to see this effort to study and improve model use and management in OSWER programs, and endorses the eventual extension of the proposed pilot project to consider model use throughout the EPA.

and support engineers and scientists with modeling development and applications skills. The Subcommittee commends this systematic effort to gather and report information on the use of models by the OSWER program, and finds that the conclusions drawn in the report are consistent with the data and information presented. The Subcommittee recommends some specific ways in which the report can be improved, including:

- a. A brief summary of the Phase I report should be included in the Phase II report.
- b. OSWER and its contractors should review the list of models for accuracy of classifications and names. In particular, some models which are known by multiple names or acronyms appear to have separate listings for each of the names. This should be corrected.
- c. The draft report indicates that "...there have been relatively few incidents of model abuse or mismanagement in the hazardous waste and Superfund program..." Further discussion of what constitutes model abuse or mismanagement is needed, as well as discussion of the factual basis for concluding that some, though little, of this has occurred.

It is also recommended that follow-up work be conducted to improve the overall value of the study for characterizing model use in hazardous waste/Superfund programs. The recommended activities and rationale include:

- a. Conducting several case studies illustrating how models were used and applied by EPA personnel. How were particular models selected and justified for a given application? What difficulties were encountered in trying to use the models? What protocol was followed in the application of the models, particularly regarding peer review of the model formulation, code validation, site-specific validation of the model application and input parameters and model sensitivity and uncertainty analysis? Finally, did the program office get the results and information they were seeking from the model application; did the model results contribute to the ultimate regulatory decision in an effective and timely manner? The case studies could be developed by reviewing the regional office interviews and conducting follow-up interviews to supplement the information. The insights gained from the case studies should be very, useful to the Agency for identifying common trends and concerns.

The difficulty with the proposed project arises from the limited and preliminary nature of mathematical models for the soil contamination problem. This is due to limited scientific understanding of the physical, chemical and biological processes which influence the level of soil contamination in the unsaturated zone. Considerable research on the soil pollution problem is currently taking place and involves studies of multiphase interactions, vapor phase transport, surface wetting phenomena, complex surface chemistry, and biological growth and uptake in alternatively oxidative and reductive environments. As such, models which can reliably predict levels of soil contamination are still very much in the research phase. As an example, Pennell et al. (1990) found that even for the relatively simple, well-studied case of aldicarb and bromide transport from the top layer of an agricultural field site, "None of the models (CMLS, MOUSE, PRZM, GLEAMS or LEACHMP) accurately described measured solute concentration distributions." Soil contamination problems at Superfund sites are often much more complex than the pesticide application problem examined in the above referenced study of Pennell et al. (1990). Hence, it will be difficult to obtain a broad consensus as to what constitutes an' acceptable model or set of models for a soil pollution problem. This does not imply that the study and field validation of soil contamination models is not of vital importance to EPA, but rather that this application area may not be appropriate for a pilot project on model administration.

As an alternative to a pilot project on soil contamination models, the Subcommittee suggested that OSWER consider a study on the use of ground water flow models, with possible extension to solute transport models applied to the saturated zone. Ground water flow models have been used in a wide range of applications for a number of years, and several good models are widely accepted as standard tools.(NRC, 1990). Problems occur in identifying appropriate dimensionality and estimating parameter values for a particular site application, especially when there is a high degree of heterogeneity in the aquifer (now recognized to be the rule, rather than the exception), and when fractured media are present. As such, there is a fair degree of uncertainty present as to which model to choose and how to parameterize it in a given application, but it is far less than the fundamental uncertainty in physical principles and basic processes which surround the formulation of unsaturated zone soil pollution models.

The Subcommittee discussed at length the benefits and tradeoffs involved in conducting 1) a pilot study in the newly developing area of soil contamination vs. 2) a study of models in a more mature area with a longer history of model development and testing, such as ground water flow models. The former alternative would require extensive scientific research investigate processes and test the basic assumptions of models. It would also test the ability to guide model use in a domain with rapidly evolving knowledge, and this often occurs in regulatory problems. The latter alternative would allow a greater focus on administrative issues, including:

APPENDIX A - THE CHARGE TO THE SUBCOMMITTEE

CONCEPT OF THE PROPOSED PILOT MODELLING PROJECT

Background

The Office of Solid Waste and Emergency Response (OSWER) management has been concerned with the growing use of computerized environmental models to support decision-making in the hazardous waste and Superfund programs. Echoing a finding in the Science Advisory Board's Modeling Resolution, OSWER is addressing the need for systematic management of model review, selection and application.

The OSWER Information Management Staff has documented the modeling activities within the Agency, particularly within the office of Research and Development, and documented model use with the regional hazardous waste and Superfund programs. Its draft "Report on the Usage of Computer Models in Hazardous Waste/Superfund Programs" contains recommendations for action in five areas. Those conclusions and their sections in the Report are:

1. training in general modelling concepts (section 4.2);
2. policy statement regarding the use of models (4.5);
3. dissemination of information on acceptable models (4.3);
4. technical support (4.4);
5. Agencywide authority for determining standards for model development, verification, validation, and review/approval procedures. (4.5)

Purpose

The following proposed pilot project addresses two of the recommendations above. There is a need for some initial experience in identifying a number of models which are "acceptable" for use, in order to disseminate that information to the potential users (3. above). There is also a need for some initial experience in determining the criteria for reviewing models for "acceptability" as a prototype for the eventual Agencywide standards (5. above).

Description of Pilot Project

The major activity of the pilot will be to review computerized models for only one area of concern to OSWER (e.g. soil transport and fate). It will be useful to limit the review to an area of modelling where acceptable models are believed to exist and for which the number of existing models is a manageable number for review purposes.

An ad hoc advisory committee will be established to provide guidance to and oversight of the project. If soil transport and

QUESTIONS FOR MEMBERS OF THE SCIENCE ADVISORY BOARD
ON THE CONCEPT OF THE PROPOSED PILOT MODELLING PROJECT

The Office of Solid Waste and Emergency Response (OSWER) has written the draft "Report on the Usage of Computer Models in Hazardous Waste/Superfund Programs". It documents the results of information gathering regarding the selection and use of models. It also includes conclusions based on the findings.

Questions on the Report

1. Based on the findings in Chapters 2 and 3, do you agree that the conclusions in Chapter 4 are basically correct?
2. Do you believe the issues regarding model selection and use are important enough to warrant the implementation of a number of recommendations?

One such recommendation has led to this proposal for a pilot project which would be directed by OSWER and would have participants from the hazardous waste and Superfund programs at headquarters and in the regions. ORD laboratories and other media offices, as well as the Office of Information Resources Management, would also participate. The purpose of the pilot project is to identify a group of models which serve a particular function and to determine the criteria which would qualify them as acceptable for use. Information concerning the models, as well as technical contacts, would be disseminated to staff in OSWER programs in the regions and at headquarters.

Questions on the Concept of the Proposed Pilot Modelling Project

1. Is the scope (a core set of models) reasonable?
2. Are the products of the pilot project (core set of models, criteria, procedures, and model information) feasible?
3. Would the products be useful for defining the mission, charter and action plan for the Agencywide modeling group? (See Report, Section 4.5.)
4. Would the products have a beneficial effect on the selection and use of models for the application area (soil transport) by regional and headquarters waste management programs?
5. What suggestions do you have regarding: selection of an initial set of models; participants in the ad hoc advisory Committee; information gathering to support the development of the criteria; other?
6. Would you be willing to consult with OSWER on the results (products) of the pilot project?

APPENDIX C - REFERENCES CITED

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